Scaling properties of net information measures for superpositions of power potentials: Free and spherically confined cases

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Abstract

The dimensional analyses of the position and momentum variances based quantum mechanical Heisenberg uncertainty measure, along with several entropic information measures are carried out for the superposition of the power potentials of the form $V(r) = Z r^n + \sum_i Z_i r^{n_i}$ where $Z, Z_i, n, n_i$ are parameters yielding bound states for a particle of mass $M$. The uncertainty product and all other net information measures for given values of the parameters $Z, Z_i$, are shown to depend only on $M$ and the ratios $Z_i/Z(Z_i^{(n_i+2)}/(n+2))$. Under the imposition of a spherical impenetrable boundary of radius $R$ over the polynomial potential, an additional parametric dependence on $R Z^{1/(n+2)}$ is derived. A representative set of numerical results are presented which support the validity of such a general scaling property.

Keywords: Heisenberg uncertainty relation; Shannon entropy; Fisher information measure; Rényi entropy; Tsallis entropy; Power potentials; Polynomial potentials; Spherically confined system

1. Introduction

The uncertainty relations are the basic properties of quantum mechanics. In particular, we have the Heisenberg uncertainty principle \footnote{1} for the product of the uncertainties in position and momentum, expressed in terms of Planck’s constant. For a one-dimensional system defined over $-\infty \leq x \leq \infty$, it is given by the product of the corresponding variances, $(\Delta x) = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$, and $(\Delta p) = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$, according to

$$ (\Delta x)(\Delta p) \geq \frac{1}{2} \hbar. \quad (1) $$

The Heisenberg uncertainty product (HUP), $(\Delta x)(\Delta p)$, has many interesting properties for different potentials. For example, HUP for the bound states in homogeneous, power potentials is independent of the strength of the potentials \footnote{2}. For several other numerical studies on HUP we refer to the published literature \footnote{3}. For such potentials similar interesting related properties are also displayed \footnote{4} through the various information measures such as the Shannon information entropy sum \footnote{5–8}, the Fisher information product \footnote{9–12}, Onicescu energy \footnote{13}, Rényi \footnote{14,15}, and Tsallis entropy \footnote{16,17}, respectively. In this Letter we will consider some general scaling properties for the bound states arising out of the superpositions of power potentials of the form

$$ V(r) = Z r^n + \sum_i Z_i r^{n_i}, \quad (2) $$

where $Z, Z_i, n, n_i$ are parameters ($n, n_i$ may not be integers), in which there are bound states for a particle of mass $M$. Specifically, in addition to the Lennard–Jones type isotropic potentials, we have

$$ V_1(r) = -\lambda r^2 + \lambda r^4 \quad (3) $$

for a symmetric double well potential \footnote{18},

$$ V_2(r) = \frac{1}{2} \lambda r^2 + \frac{a}{r^2} \quad (4) $$

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2. Dimensionality and uncertainty relations

In this section we shall derive some dimensionality properties and discuss their implications on the uncertainty relations for the bound states resulting from superpositions of the isotropic power potentials.

The basic dimensional parameters in our Schrödinger equation in Eq. (6) are $\hbar^2 / M$, $Z$, $Z_i$. Of these,

$$s_i = \frac{M}{\hbar^2 Z_i} \left( \frac{\hbar^2}{MZ} \right)^{\frac{1}{n+2}}$$

are the dimensionless parameters. Now we consider the standard deviations

$$\langle \Delta r \rangle^2 = \langle \vec{r}^2 \rangle - \langle \vec{r} \rangle^2 = \langle \vec{p}^2 \rangle - \langle \vec{p} \rangle^2.$$  

For our potential in Eq. (2), the dimensionality properties imply that the deviations are of the form

$$\Delta r = \frac{\hbar^2 / M Z}{\hbar^2 / M Z} g_1(s_i),$$

$$\Delta \vec{p} = \hbar \left( \frac{M Z / \hbar^2}{M Z} \right)^{1/(n+2)} g_2(s_i).$$

so that the uncertainty product is

$$\Delta r \Delta \vec{p} = \hbar g_1(s_i) g_2(s_i), \quad s_i = \frac{M}{\hbar^2} Z_i \left( \frac{\hbar^2}{MZ} \right)^{\frac{n+2}{n+2}}.$$  

This implies that the HUP depends only on the dimensionless parameters $s_i$. The quantity $s_i$, according to Eq. (7) includes $M$ and in general HUP depends on $M$. Our numerical results presented in Section 4 are reported in a.u. whereby it is implied that $M = 1$. Under this assumption, the parameter $s_i$ would be completely characterized by $Z_i / Z(n+2)/(n+2)$. Thus, for the potential $V_1(r)$ in Eq. (3), HUP depends only on $\lambda r^{-3/2}$, and for the potential $V_2(r)$ in Eq. (4), it depends only on $a$. It may also be noted that the bound state energies are of the form

$$E = \left( \frac{\hbar^2}{M} \right)^{n/(n+2)} Z^{2/(n+2)} g_3(s_i).$$

These results follow from just the dimensionality properties of the parameters and the exact expressions of $g_i(s_i)$ in Eqs. (9)–(11) are not obtained.

3. Scaling properties of net information measures

We will now consider some scaling properties for bound states in a superposition of power potentials, and their implications for Shannon entropy and other properties.

3.1. Scaling properties

For the Schrödinger equation in Eq. (6), the energy $E$ and eigenfunction $\psi$ are functions of the form

$$E: \ E \left( \frac{\hbar^2}{M}, Z, Z_i \right), \quad \psi: \ \psi \left( \frac{\hbar^2}{M}, Z, Z_i, r \right).$$

Multiplying Eq. (6) by $\hbar^2 / M$, and introducing a scale transformation

$$\vec{r} = \lambda \vec{r}$$

one gets

$$\frac{1}{2} \nabla^2 \psi + \left( \frac{M}{\hbar^2} \right) \left[ Z \lambda^{n+2} r^m + \sum Z_i \lambda^{n_i+2} r_i^{m_i} \right] \psi = \left( M / \hbar^2 \right) \lambda^2 E \psi.$$  

Taking

$$\lambda = \left( \frac{\hbar^2}{MZ} \right)^{1/(n+2)},$$

it leads to

$$\frac{1}{2} \nabla^2 \psi + \frac{M}{\hbar^2} \sum Z_i \left( \frac{\hbar^2}{MZ} \right)^{\frac{n_i+2}{n+2}} r_i^{m_i} \psi = M \left( \frac{\hbar^2}{MZ} \right)^{2/(n+2)} E \psi.$$  

Comparing this with Eq. (6), we obtain

$$E \left( \frac{\hbar^2}{M}, Z, Z_i \right) = \left( \frac{\hbar^2}{M} \right) \lambda^{-2} E \left( 1, 1, Z, Z_i \lambda^{n_i+2} M / \hbar^2 \right),$$

for a modified isotropic harmonic oscillator [19], and

$$V_3(r) = -\frac{Z}{r} + \lambda r$$

for a confined hydrogenic system [20] and the static quarkonium potential [21]. The Schrödinger equation for the potential in Eq. (2) is

$$-\frac{\hbar^2}{2M} \nabla^2 \psi + \left[ Z r^n + \sum Z_i r_i^{m_i} \right] \psi = E \psi.$$  

We note here that the generalized cosine exponential screened Coulomb potentials [22] which are the natural extensions of the Yukawa [23] and Hulthén [24] potentials can be expressed, to a good approximation, as polynomial potentials [18–21,25,27–29] several numerical studies dealing with the eigenvalue spectrum have been reported previously [30,31]. For the sake of clarity of presentation this Letter is structured as follows. In Section 2, some general properties corresponding to the Heisenberg uncertainty product, HUP, are derived for the potential $V(r)$. In Section 3, the scaling property of the associated position and momentum space densities is derived following which it is shown how the scaling property of the Shannon information entropy sum [5–8], the Fisher information product [9] and other information measures [13,14,16] can be obtained from it. Further, in Section 3 we have considered the scaling properties of the potential $V(r)$ under the specific condition of confinement inside an impenetrable spherical boundary wall defined by a radius $R$. In Section 4, we present numerical results, in atomic units, which support the analytic results derived in this work. Finally, a summary of the main results is presented in Section 5.
\[ \lambda = \left( \frac{h^2}{MZ} \right)^{1/(n+2)}, \]
\[ \psi \left( \frac{h^2}{M}, Z, Z_i, r \right) = A \psi \left( 1, 1, Z_i \lambda^{n_i+2} M / h^2, r' \right), \quad r = \lambda r'. \] (17)

Taking \( \psi \left( 1, 1, Z_i \lambda^{n_i+2} M / h^2, r' \right) \) to be normalized, the normalization of the wave function \( \psi(h^2/M, Z, Z_i, r) \) leads to
\[ 1 = A^2 \int \left| \psi \left( 1, 1, Z_i \lambda^{n_i+2} M / h^2, r' \right) \right|^2 d^3 r = A^2 \lambda^3, \Rightarrow A = \lambda^{-3/2} = \left( MZ/h^2 \right)^{3/(n+2)}, \] (18)
so that
\[ \psi \left( \frac{h^2}{M}, Z, Z_i, r \right) = \lambda^{-3/2} \psi \left( 1, 1, Z_i \lambda^{n_i+2} M / h^2, r' \right), \]
\[ \lambda = \left( \frac{h^2}{MZ} \right)^{1/(n+2)}, \quad r' = r/\lambda. \] (19)

For obtaining the wave function in the momentum space, we take the Fourier transform of the wave function in Eq. (19), leading to
\[ f \left( \frac{h^2}{M}, Z, Z_i, p \right) = \frac{1}{(2\pi h)^3} \int d^3 r e^{-i\vec{p} \cdot \vec{r}/h} \psi \left( \frac{h^2}{M}, Z, Z_i, r \right). \] (20)

Using the relation in Eq. (19) and changing the integration variable to \( r' \), we get
\[ f \left( \frac{h^2}{M}, Z, Z_i, p \right) = \lambda^{3/2} f \left( 1, 1, Z_i \lambda^{n_i+2} M / h^2, p' \right), \]
\[ \lambda = \left( \frac{h^2}{MZ} \right)^{1/(n+2)}, \quad p' = \lambda p. \] (21)

From the relations in Eqs. (19)-(20), one has for the corresponding position and momentum densities,
\[ \rho \left( \frac{h^2}{M}, Z, Z_i, r \right) = \lambda^{-3} \rho \left( 1, 1, s_i, r' \right), \]
\[ \gamma \left( \frac{h^2}{M}, Z, Z_i, p \right) = \lambda^3 \gamma \left( 1, 1, s_i, p' \right), \]
\[ \lambda = \left( \frac{h^2}{MZ} \right)^{1/(n+2)}, \quad s_i = \lambda^{n_i+2}MZ_i/h^2, \]
\[ r' = r/\lambda, \quad p' = \lambda p, \] (22)
with \( s_i \) being the scaled parameters.

### 3.2. Net Shannon information entropy

The Shannon entropies in the position and momentum space are,
\[ S_r = - \int \rho(r) \ln \rho(r) \, d^3r, \]
\[ S_p = - \int \gamma(p) \ln \gamma(p) \, d^3p. \] (23)

Using the relations in Eq. (22), we get for these entropies
\[ S_r (\frac{h^2}{M}, Z, Z_i) = 3 \ln \lambda + S_r (1, 1, s_i), \]
\[ S_p (\frac{h^2}{M}, Z, Z_i) = -3 \ln \lambda + S_p (1, 1, s_i), \] (24)
which imply that the Shannon entropy sum \( S_T = S_r + S_p \) satisfies the relation
\[ S_T (\frac{h^2}{M}, Z, Z_i) = S_T (1, 1, s_i), \]
\[ s_i = \frac{M}{h^2} Z_i \left( \frac{h^2}{MZ} \right)^{\frac{n_i+2}{n+2}}. \] (25)

Therefore, for given values of the parameters \( Z, Z_i \), the Shannon entropy sum depends only on the ratios \( Z_i/Z(n_i+2)/(n+2) \).

### 3.3. Net Fisher information measure

The Fisher information measures for position and momentum are
\[ I_r = \int \frac{[\nabla \rho(r)]^2}{\rho(r)} \, d^3r, \quad I_p = \int \frac{[\nabla \gamma(p)]^2}{\gamma(p)} \, d^3p. \] (26)

Using the relations in Eq. (22), one obtains
\[ I_r (\frac{h^2}{M}, Z, Z_i) = \frac{1}{\lambda^2} I_r (1, 1, s_i), \]
\[ I_p (\frac{h^2}{M}, Z, Z_i) = \lambda^2 I_p (1, 1, s_i), \] (27)
which together imply that the Fisher information product \( I_r I_p \) satisfies the relation
\[ I_{rp} (\frac{h^2}{M}, Z, Z_i) = I_{rp} (1, 1, s_i), \]
\[ I_{rp} = I_r I_p, \quad s_i = \frac{M}{h^2} Z_i \left( \frac{h^2}{MZ} \right)^{\frac{n_i+2}{n+2}}. \] (28)

Here, for given values of the parameters \( Z, Z_i \), the Fisher information product depends only on the ratios \( Z_i/Z(n_i+2)/(n+2) \). In particular, for the potential \( V_1(r) \) in Eq. (3), it depends only on \( \lambda k^{-3/2} \), and for the potential \( V_2(r) \) in Eq. (4), it depends only on \( a \). We note here that the universal lower bound [6] on \( S_r \) has been widely studied in the literature [7,8].

### 3.4. Rényi entropy

The Rényi entropies in position and momentum spaces are
\[ H_{\alpha}^{(r)} = \frac{1}{1-\alpha} \ln \int \rho(r)^\alpha \, d^3r, \]
\[ H_{\alpha}^{(p)} = \frac{1}{1-\alpha} \ln \int \gamma(p)^\alpha \, d^3p. \] (29)

With the relations in Eq. (22), we get for these entropies,
\[ H_{\alpha}^{(r)} (\frac{h^2}{M}, Z, Z_i) = 3 \ln \lambda + H_{\alpha}^{(r)} (1, 1, s_i), \]
\[ H_{\alpha}^{(p)} (\frac{h^2}{M}, Z, Z_i) = -3 \ln \lambda + H_{\alpha}^{(p)} (1, 1, s_i), \] (30)
which imply that the Rényi entropy sum \( H_{\alpha}^{(T)} = H_{\alpha}^{(r)} + H_{\alpha}^{(p)} \) satisfies the relation
\[ H_{\alpha}^{(T)} \left( \frac{h^2}{M}, Z, Z_i \right) = H_{\alpha}^{(T)} (1, 1, s_i), \]
\[ s_i = \frac{M}{h^2} Z_i \left( \frac{h^2}{MZ} \right)^{\frac{n_i+2}{n+2}}. \] (31)
Therefore, as in other cases, for given values of the parameters \( Z, Z_i \), the Rényi entropy sum depends only on the ratios \( Z_i/Z^{(n_i+2)/(n+2)} \). In particular, for the potential \( V_1(r) \) in Eq. (3), it depends only on \( \lambda k^{-3/2} \), and for the potential \( V_2(r) \) in Eq. (4), it depends only on \( a \). We note here that interesting lower bounds involving Rényi entropies have been recently proposed [15].

3.5. Onicescu energies

The Onicescu energies in position and momentum spaces are

\[
E_r = \int [\rho(r)]^2 d^3 r, \quad E_p = \int [y(p)]^2 d^3 p. \tag{32}
\]

Using the relations in Eq. (22), we get

\[
E_r (h^2/M, Z, Z_i) = \frac{1}{\lambda^4} E_r (1, 1, s_i),
\]

\[
E_p (h^2/M, Z, Z_i) = \lambda^3 E_p (1, 1, s_i), \tag{33}
\]

which imply that the Onicescu energy product \( E_{rp} = E_r E_p \) satisfies the relation

\[
E_{rp} (h^2/M, Z, Z_i) = E_{rp} (1, 1, s_i),
\]

\[
s_i = \frac{M}{\hbar^2 Z_i} \left( \frac{h^2}{MZ} \right)^{\frac{2}{n+2}}. \tag{34}
\]

In this case also, for given values of the parameters \( Z, Z_i \), the Onicescu energy product depends only on the ratios \( Z_i/Z^{(n_i+2)/(n+2)} \). In particular, for the potential \( V_1(r) \) in Eq. (3), it depends only on \( \lambda k^{-3/2} \), and for the potential \( V_2(r) \) in Eq. (4), it depends only on \( a \).

3.6. Tsallis entropy

The Tsallis entropies in position and momentum spaces are

\[
T_r = \frac{1}{q-1} \left[ 1 - \int [\rho(r)]^q d^3 r \right],
\]

\[
T_p = \frac{1}{m+1} \left[ 1 - \int [y(p)]^m d^3 p \right]. \tag{35}
\]

We consider the integral terms

\[
J_r (h^2/M, Z, Z_i) = \int [\rho(r)]^q d^3 r,
\]

\[
J_p (h^2/M, Z, Z_i) = \int [y(p)]^m d^3 p. \tag{36}
\]

Using the relations in Eq. (22), we get

\[
J_r (h^2/M, Z, Z_i) = \lambda^{3q-3} J_r (1, 1, s_i),
\]

\[
J_p (h^2/M, Z, Z_i) = \lambda^{3m-3} J_p (1, 1, s_i). \tag{37}
\]

Then one obtains for the ratio

\[
J_{r/p} (h^2/M, Z, Z_i) = J_{p/r} (1, 1, s_i),
\]

\[
s_i = \frac{M}{\hbar^2 Z_i} \left( \frac{h^2}{MZ} \right)^{\frac{q}{n+2}}.
\]

\[
J_{p/r} = \frac{J_p^{1/2m}}{J_r^{1/2q}}, \quad \frac{1}{m} + \frac{1}{q} = 2. \tag{38}
\]

Therefore in this case also, for given values of the parameters \( Z, Z_i \), the ratio of Tsallis entropies depends only on the ratios \( Z_i/Z^{(n_i+2)/(n+2)} \). In particular, for the potential \( V_1(r) \) in Eq. (3), it depends only on \( \lambda k^{-3/2} \), and for the potential \( V_2(r) \) in Eq. (4), it depends only on \( a \). We note here that the lower bounds associated with the net Tsallis entropy have been studied in the literature [17].

3.7. Spherically confined potential

We shall consider here the case of polynomial potential in Eq. (2) in the presence of a superposition potential due to an impenetrable spherical cavity of radius \( R \). Along with the parameters as obtained in Eq. (10), \( s_i = (h^2/M)^{(n_i-n)/(n+2)} Z_i/Z^{(n_i+2)/(n+2)} \), we now have an additional dimensionless parameter \( s = (M/\hbar^2)^{(1/(n+2)} RZ^{1/(n+2)} \). For the special case of \( n = -1, s \) reduces to \( RZ \). An interesting case is of confined \( a/r^2 \). In this case, the only dimensionless parameter is \( s = (h^2/Ma) \). So the uncertainty relation and the net information measures depend only on \( s \) and are independent of \( R \). It also implies that for a particle in a spherical box (\( a = 0 \)), the information products are independent of \( R \). We conclude this section by noting that under the similarly confined conditions the other net information measures considered by us also depend only on the scaled parameters \( s_i \) and \( s \).

4. Numerical results

For a few specific cases of \( V(r) \), e.g. Eq. (4), analytic solutions can be found. In principle, the scaling properties which are proven in the preceding sections can be ascertained using such solutions. However, our analysis on the basis of general dimensional and scaling properties are valid for the bound states of \( V(r) \) with analytical, semi-analytical or numerical solutions. In this section we present some representative set of computational results in order to test the analytic results derived in Section 3. For the general potential \( V(r) \) in Eq. (2), we have chosen the five-term polynomial potentials from the literature [30]. In particular the potentials used therein at serial number 1–8 and 37–40 have been considered by us,

\[
V(r) = Z/r + Z_1 r + Z_2 r^2 + Z_3 r^3 + Z_2 r^4. \tag{39}
\]

We have generated the momentum space wave function through Fourier transformation of the position space wave function [2, 4,32] and the corresponding densities were used to compute the square of HUP as \( \langle r^2 \rangle \langle p^2 \rangle \).

In Table 1, the squares of HUP given by Eq. (1) corresponding to the potentials \( V(r) \) are presented for a set of parameters \( [Z, Z_i] \) as displayed in columns 2–5 for the values of \( n = -1 \), and \( n_1, n_2, n_3 \), and \( n_4 \) are given by 1, 2, 3, and 4, respectively. For the spherical potentials considered here, the square of HUP is given by the product \( \langle r^2 \rangle \langle p^2 \rangle \). For each potential
where we have considered a suitably scaled set of parameters to generate another polynomial potential from it such that the ratios $Z_i/Z^{(n+2)}$ are held fixed for such a pair of potentials. The constancy of the values of $(r^2)/(p^2)$ shown in the last column confirms numerically the invariance of HUP with respect to the constant values of the ratios $Z_i/Z^{(n+2)}$ in case of all the 12 potentials considered in Table 1. It is noteworthy that the selection of the polynomial potentials covers the range $I = 0–3$ values. Our last numerical test concerns with the spherically confined polynomial potential. In Table 2, rows 2 and 5, we have considered the polynomial potentials of the form given by Eq. (39) with the coefficients taken as those reported at serial numbers 2 and 5 of the earlier work [30] and have imposed upon them the spherical confining potential with impenetrable boundaries [32]. The radius of the sphere is given by $R$.

As representative examples of the net information entropy, we show the numerical results corresponding to the position and momentum space Shannon entropy along with the net Shannon entropy values in columns 7–9, respectively. For each potential, with a given set of parameters $[Z, Z_i]$ and $R$ we have generated two more potentials [rows 3–4 and 6–7] such that the quantities $Z_i/Z^{(n+2)}$ and $RZ$ are held fixed. The numerical results of the corresponding net Shannon entropies are found to be invariant under such a scaling of the parameters defining the polynomial potential $V(r)$. A similar conclusion can be drawn from the numerical results obtained for the Onicescu energy values $E_r$, $E_p$ and $E_{rp}$ shown in the last three columns, Table 2. We note here that the analytic results obtained in this work for the other entropic measures have been extensively tested numerically by us and they provide results showing similar agreement in terms of the scaling properties as given by Tables 1–2.
5. Summary

In this Letter we have carried out the dimensional analyses of the position and momentum variance based quantum mechanical Heisenberg uncertainty measure, along with several entropic information measures corresponding to the bound states determined by the superposition of the power potentials of the form \( V(r) = Zr^n + \sum Z_i r^{n_i} \) where \( Z, Z_i, n, n_i \) are parameters yielding bound states for a particle of mass \( M \). The uncertainty product and all other net information measures for given values of the parameters \( Z, Z_i \), are found to be functions of the parameters \( Z_i/Z^{(n_i+2)/(n+2)} \). With the imposition of a spherical impenetrable boundary of radius \( R \) on the polynomial potential, an additional parametric dependence on \( RZ^{1/(n+2)} \) is derived. A representative set of numerical results are presented which support the validity of such a general scaling property. In view of the widespread utility of the polynomial potentials, the results reported here could be used to benchmark the approximate methods of calculations of the wave functions corresponding to such potentials. An interesting result in the case of the confined potential is the existence of an extremum for the net information measures considered here as a function of \( R \), the confining radius. Further, the scaling of this location, \( R_m \) of extremum is precisely given by \( RZ^{1/(n+2)} \). For the hydrogen-like atoms, for example, \( R_m \) scales as \( 1/Z \), just like the location of the radial node of the free hydrogen-like atoms.

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